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References

- [1] Takeshi Nishimatsu, Umesh V. Waghmare, Yoshiyuki Kawazoe, and David Vanderbilt. Fast molecular-dynamics simulation for ferroelectric thin-film capacitors using a first-principles effective hamiltonian. *Phys. Rev. B*, 78:104104, Sep 2008.
- [2] Jaita Paul, Takeshi Nishimatsu, Yoshiyuki Kawazoe, and Umesh V. Waghmare. Ferroelectric phase transitions in ultrathin films of BaTiO_3 . *Phys. Rev. Lett.*, 99:077601, Aug 2007.
- [3] Takeshi Nishimatsu, Masaya Iwamoto, Yoshiyuki Kawazoe, and Umesh V. Waghmare. First-principles accurate total energy surfaces for polar structural distortions of BaTiO_3 , PbTiO_3 , and SrTiO_3 : Consequences for structural transition temperatures. 82(13):134106.
- [4] Takeshi Nishimatsu, Masaya Iwamoto, Yoshiyuki Kawazoe, and Umesh V. Waghmare. First-principles accurate total energy surfaces for polar structural distortions of BaTiO_3 , PbTiO_3 , and SrTiO_3 : Consequences for structural transition temperatures. 82(13):134106.

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